The analyticity region of the hard sphere gas. Improved bounds

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Abstract

We find an improved estimate of the radius of analyticity of the pressure of the hard-sphere gas in d dimensions. The estimates are determined by the volume of multidimensional regions that can be numerically computed. For $d = 2$, for instance, our estimate is about 40% larger than the classical one.

In a recent paper [4] two of us have shown that it is possible to improve the radius of convergence of the cluster expansion using a tree graph identity due to Penrose [2], see also [5, Section 3]. In this short letter we use the same idea to improve the estimates of the radius of analyticity of the pressure of the hard-sphere gas.

The grand partition function $\Xi(z,\Lambda)$ of a gas of hard spheres of diameter R enclosed in a volume $\Lambda \subset \mathbb{R}$ is given by

$$\Xi(z,\Lambda) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} dx_1 ... dx_n \, \exp\Big\{ - \sum_{1\le i<j\le n} U(x_i - x_j) \Big\}$$

with

$$U(x-y) = \begin{cases} 0 & \text{if } |x-y| > R \\ +\infty & \text{if } |x-y| \le R \end{cases}$$

where $|x-y|$ denotes the euclidean distance between the sphere centers x and y. The corresponding pressure is $\lim_{\Lambda\to\mathbb{R}^d} P(z,\Lambda)$ (limit in van Hove sense), where

$$P(z,\Lambda) \;=\; \frac{1}{|\Lambda|} \log \Xi(z,\Lambda)$$

($|\Lambda|$ denotes the volume of the region Λ). The cluster expansion, in this setting, amounts to writing the preceding logarithm as the power series (see e.g. [1])

$$\log \Xi(z,\Lambda) = \sum_{n=1}^{\infty} \frac{z^n}{n!} \int_{\Lambda^n} dx_1 ... dx_n \sum_{\substack{g \subset g(x_1,....x_n) \\ g \in G_n}} (-1)^{|g|} \tag{1}$$

where the graph $g(x_1,....x_n)$ has vertex set $\{1,...,n\}$ and edge set $E(x_1,....x_n) = \{\{i,j\} : |x_i - x_j| \le R\}$ (that is, if the spheres centered at x_i and x_j intersect), G_n is the set of all the connected graphs with vertex set $\{1,...,n\}$, and $|g|$ denotes the cardinality of the edge set of the graph g. Only families $(x_1,....x_n)$ for which $g(x_1,....x_n)$ is connected contribute to (1); such families represent "clusters" of spheres.

The standard way to estimate the radius of analyticity of the pressure is to obtain a Λ-independent lower bound of the radius of convergence of the series

$$|P|(z,\Lambda) \;=\; \frac{1}{|\Lambda|} \sum_{n=1}^{\infty} \frac{|z|^n}{n!} \int_{\Lambda^n} dx_1 ... dx_n \left| \sum_{\substack{g \subset g(x_1,....x_n) \\ g \in G_n}} (-1)^{|g|} \right| . \tag{2}$$

This strategy leads to the classical estimation (see e.g. [6], Section 4) that the pressure is analytic if

$$|z| \;<\; \frac{1}{e\, V_d(R)} \;, \tag{3}$$

where $V_d(R)$ is the volume of the d-dimensional sphere of radius R (excluded volume).

Our approach is based on a well known tree identity. Let us denote by T_n the subset of G_n formed by all tree graphs with vertex set $\{1,...,n\}$. Given a tree $\tau \in T_n$ and a vertex i of τ, we denote by d_i the *degree* of the vertex i in τ, i.e. the number of edges of τ containing i. We regard the trees $\tau \in T_n$ as rooted in the vertex 1. This determines the usual partial order of vertices in τ by generations: If u, v are vertices of τ, we write $u \prec v$ —and say that u precedes v— if the (unique) path from the root to v contains u. If $\{u,v\}$ is an edge of τ, then either $v \prec u$ or $u \prec v$. Let $\{u,v\}$ be an edge of τ and assume without loss of generality that $u \prec v$, then u is the called the *predecessor* and v the *descendant*. Every vertex $v \in \tau$ has a unique predecessor and $s_v = d_v - 1$ descendants, except the root that has no predecessor and $s_v = d_v$ descendants. For each vertex v of τ we denote by v' the unique predecessor of v and by $v^1, \dots v^{s_v}$ the s_v descendants of v. The number s_v is called the branching factor; vertices with $s_v = 0$ are called end-points or "leaves".

Penrose [4] showed that the sum in (1) is equal, up to a sign, to a sum over trees satisfying certain constraints. We shall keep only the "single-vertex" constraints: descendants of a given sphere must be mutually non-intersecting. This implies that

$$\left| \sum_{\substack{g \subset g(x_1,....x_n) \\ g \in G_n}} (-1)^{|g|} \right| \;\le\; \sum_{\tau \in T_n} w_\tau(x_1,....x_n) \tag{4}$$

where

$$w_\tau(x_1,....x_n) = \begin{cases} 1 & \text{if } |x_v - x_{v'}| \le R \text{ and } |x_{v^i} - x_{v^j}| > R, \ \forall v \text{ vertex of } \tau,\ \{i,j\} \subset \{1,\dots,s_v\}, \\ \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

Hence from (2) and (4) we get

$$|P|(z,\Lambda) \;\le\; \sum_{n=1}^{\infty} \frac{|z|^n}{n!} \sum_{\tau \in T_n} S_\Lambda(\tau) \tag{6}$$

with

$$S_\Lambda(\tau) \;=\; \frac{1}{|\Lambda|} \int_{\Lambda^n} w_\tau(x_1,....x_n)\, dx_1 ... dx_n \;. \tag{7}$$

By (5) we have

$$S_\Lambda(\tau) \;\le\; g_d(d_1) \prod_{i=2}^{n} g_d(d_i - 1) \tag{8}$$

where d_i is the degree of the vertex i in τ,

$$g_d(k) \;=\; \int_{\substack{|x_i| \le R \\ |x_i - x_j| > R}} dx_1 \ldots dx_k \;=\; R^{dk} \int_{\substack{|y_i| \le 1 \\ |y_i - y_j| > 1}} dy_1 \ldots dy_k$$

for k positive integer, and $g_d(0) = 1$ by definition. It is convenient to write

$$g_d(k) \;=\; [V_d(R)]^k \, \widetilde{g}_d(k) \tag{9}$$

with

$$\widetilde{g}_d(k) \;=\; \frac{1}{[V_d(1)]^k} \int_{\substack{|y_i| \le 1 \\ |y_i - y_j| > 1}} dy_1 \ldots dy_k \tag{10}$$

for k positive integer and $\widetilde{g}_d(0) = 1$. We observe that $\widetilde{g}_d(k) \le 1$ for all values of k. From (8)–(10) we conclude that

$$\begin{aligned}
S_\Lambda(\tau) \quad &\le \quad [V_d(R)]^{d_1} \, \widetilde{g}_d(d_1) \prod_{i=2}^{n} [V_d(R)]^{d_i - 1} \, \widetilde{g}_d(d_i - 1) \\
&= \quad [V_d(R)]^{n-1} \, \widetilde{g}_d(d_1) \prod_{i=2}^{n} \widetilde{g}_d(d_i - 1) \; .
\end{aligned}$$

The last identity follows from the fact that for every tree of n vertices, $d_1 + \cdots + d_n \,=\, 2n - 2$. The τ-dependence of this last bound is only through the degree of the vertices, hence it leads, upon insertion in (6), to the inequality

$$|P|\,(z,\Lambda) \;\le\; \frac{1}{V_d(R)} \sum_{n=1}^{\infty} \frac{\big(|z|\, V_d(R)\big)^n}{n!} \sum_{\substack{d_1,\ldots,d_n \\ d_1+\ldots+d_n = 2n-2}} \widetilde{g}_d(d_1) \prod_{i=2}^{n} \widetilde{g}_d(d_i - 1) \, \frac{(n-2)!}{\prod_{i=1}^{n} (d_i - 1)!} \; .$$

The last quotient of factorials is, precisely, the number of trees with n vertices and fixed degrees $d_1, \ldots, d_n$, according to Cayley formula.

At this point we can bound the last sum by a power in an obvious manner. The convergence condition so obtained would already be an improvement over the classical estimate (3). We can, however, get an even better result through a trick used by two of us in [3]. We multiply and divide by a^{n-1} where $a > 0$ is a parameter to be chosen in an optimal way. This leads us to the inequality

$$\begin{aligned}
|P|\,(z,\Lambda) \quad &\le \quad \frac{a}{V_d(R)} \sum_{n=1}^{\infty} \frac{\big(|z|\, V_d(R)\big)^n}{a^n \, n(n-1)} \sum_{\substack{d_1,\ldots,d_n \\ d_1+\ldots+d_n = 2n-2}} \frac{\widetilde{g}_d(d_1)\, a^{d_1}}{d_1!} \prod_{i=2}^{n} \frac{\widetilde{g}_d(d_i - 1)\, a^{d_i - 1}}{(d_i - 1)!} \\
&\le \quad \frac{a}{V_d(R)} \sum_{n=1}^{\infty} \frac{1}{n(n-1)} \bigg(\frac{|z|}{a} [V_d(R)] \Big[\sum_{s \ge 0} \frac{\widetilde{g}_d(s) a^s}{s!} \Big] \bigg)^n
\end{aligned}$$

The last series converges if

$$|z|\, V_d(R) \;\le\; \frac{a}{C_d(a)}$$

where

$$C_d(a) \;=\; \sum_{s \ge 0} \frac{\widetilde{g}_d(s)}{s!} \, a^s$$

(this is a finite sum!). The pressure is, therefore, analytic if

$$|z|\, V_d(R) \;\le\; \max_{a>0} \frac{a}{C_d(a)}\;. \tag{11}$$

This is our new condition.

Let us show that for $d=2$ the quantitative improvement given by this condition can be substantial. In this case

$$C_2(a) \;=\; \sum_{s=0}^{5} \frac{\widetilde{g}_2(s)}{s!} a^s$$

where, by definition, $\widetilde{g}_2(0)=\widetilde{g}_2(1)=1$. The factor $\widetilde{g}_2(2)$ can be explicitly evaluated in terms of straightforward integrals and we get

$$\widetilde{g}_2(2) = \frac{3\sqrt{3}}{4\pi}$$

The other terms of the sum can be numerically evaluated using a simple Montecarlo simulation, obtaining

$$\widetilde{g}_2(3) = 0,0589 \qquad \widetilde{g}_2(4) = 0,0013 \qquad \widetilde{g}_2(5) \le 0,0001$$

Choosing $a = \left[\frac{8\pi}{3\sqrt{3}}\right]^{1/2}$ (a value for which $\frac{a}{C_d(a)}$ is close to its maximum) we get

$$|z|\, V_2(R) \;\le\; 0.5107\;.$$

This should be compared with the bound $|z|\, V_2(R) \le 0.36787\ldots$ obtained through the classical condition (3).

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